Investigation of the probability of time asymptotics of drift battery reserve in the environment with observation by traps

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Abstract

The calculation modeling of particles diffusing in environments taking into account traps in an electric field was carried out. As a result of the study, it was shown that at sufficiently large times this drift mechanism determines a new time probability of behavior. Are established depending on the characteristic time describing the exponential decrease in the number of particles, on the capacitors of the traps and on the magnitude of the stability field.

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Introduction

The problem of particle diffusion in media with absorbing traps has been studied in many papers [1-3]. The interest is due to both various applications and the analogy with the problem of the density of states in disordered media [4], as well as possible new features in particle transport [5]. In [6], the case of capture of randomly distributed in space, diffusing particles by absorbing traps was studied in detail. It was shown that the probability of particle survival $W(t;c)$ at short times $t << t_c$, where $t_c = (Dc^2)^{-1}$, (here D is the diffusion coefficient, c is the concentration of traps in the one-dimensional case) decreases exponentially:

$$W(t;c) \propto W_0 \exp\left(-\frac{t}{t_c}\right) \quad (1)$$

However, at large times, the asymptotics of the survival probability is determined by the existence of sufficiently large regions free of absorbing traps, and is of a fractional-exponential nature:

$$W(t;c) \propto W_0 \left(\frac{Dtc^2}{3\pi}\right)^{1/2} \exp\left(-\frac{3\pi^{1/2}(Dtc^2)^{1/3}}{2}\right) \quad (2)$$

Previously, in [7-9], the particle transport mechanism caused by particle drift was investigated. It was shown that at sufficiently long times, it is this mechanism that will determine the time asymptotics of the probability of particle survival in media with absorbing traps. It should be noted that in the problem of diffusion with absorbing traps, when the electric field is turned on, two new parameters additionally arise. The first of these is the "field" time, the time at which the drift displacement is compared with the diffusion: $v^2 t_E^2 \propto D t_E$, (v is the drift velocity of the particle) :

$$t_E = \frac{v^2}{D} \tag{3}$$

It is easy to understand that at times large compared to the "field" drift of particles becomes dominant. Accordingly, in sufficiently strong fields, a new asymptotic behavior was predicted for the probability of particle survival in media with absorbing traps with a characteristic time depending on the electric field strength.

In this paper, a numerical simulation of diffusion processes in media with traps in an electric field is carried out. It is shown that turning on the electric field leads to the appearance of a new characteristic "field" time. The dependence of the effective time describing the exponential decrease in the probability of survival on the electric field and the concentration of traps is studied. The dependence of the effective time on two parameters is constructed in the form of a two-dimensional surface. The article is structured as follows. Section 2 presents the main theoretical results on the effect of the electric field on particle capture. Section 3 describes the algorithm, simulation methods, including visualization of the results. Section 3 presents the results of numerical simulation. The Conclusion discusses the obtained results.

2. Diffusion in media with traps. Effect of electric field on particle capture.

Let us briefly outline the main considerations on the problem of diffusion in media with traps, leading to the result (1). According to the work [6], a solution to the standard diffusion equation is constructed:

(4)

with the following initial and boundary conditions:

$$W(x,0) = \frac{1 - c}{L} \qquad W(x_i, t) = W(x_{i+1}, t) = 0 \tag{5}$$

Here L is the length of the chain, x_i , x_{i+1} are the coordinates of the absorbing traps. This solution has the form:

$$W(x,t: x_i) = \frac{4}{L}\sum_{n=0}^{\infty} \exp\left(-\frac{Dk_n^2 t}{2}\right) \frac{\sin(k_n(x - x_i))}{k_n l_i} \tag{6}$$

Values $k_n = \frac{(2n+1)\pi}{l_i}$, $l_i = |x_{i+1} - x_i|$

The desired value is the probability of survival $W(x,t:$ $W(x,t:$ which is equal to the average value

$$\overline{W}(t) = \sum_i W(t, x_i) = \sum_i \int_{x_i}^{x_{i+1}} W(x, t; x_i)\, dx \tag{7}$$

For a random Poisson distribution of traps $f(l) = c\exp(-cl)$, where $c = \frac{N}{L}$ is the concentration of traps, l is the distance between traps, we obtain formula (1) at short times, and formula (2) at long times.

2.1. The influence of electric field on the probability of survival in environments with traps.

We include the electric field in the problem of diffusion in media with absorbing traps in a standard way. Accordingly, the diffusion equation in the electric field will take the form:

$$\frac{\partial W(x,t)}{\partial t} = D\frac{\partial^2 W(x,t)}{\partial t^2} + v\frac{\partial W(x,t)}{\partial x} \tag{8}$$

Here $v = \mu E$ is the drift velocity of particles in the electric field E, μ is the mobility of the particle. We set the initial and boundary conditions similar to the conditions (4) formulated above. Accordingly, we seek a solution in the form of an expansion in eigenfunctions:

$$W(x,t; E) = \sum_{n=0}^{\infty} c_n \varphi_n \exp(-E_n t) \tag{9}$$

where eigenfunctions are:

$$\varphi_n = \exp\left(\frac{v(x - x_i)}{2D}\right) \sin(k_n(x - x_i)) \tag{10}$$

and the eigenvalues are determined by the expression:

$$E_n = Dk_n^2 + \frac{v^2}{4D} \tag{11}$$

Accordingly, in times $t >> t_E$ we obtain an exponential decrease due to the drift of particles onto absorbing traps under the action of an electric field, corresponding to the mean field approximation:

$$\overline{W}(t; E) \propto \exp\left(-\frac{v^2 t}{4D}\right) \tag{12}$$

2.2. Accounting for fluctuations in the concentration of absorbing traps and the influence of the electric field on the fluctuation mechanism.

According to the results of [10-12], the asymptotic form of the solution depends on the magnitude of the electric field. In the case of weak fields (or small scales) $\frac{vl}{D} << 1$, we obtain the well-known result: the probability of survival is determined by fluctuations in the concentration of absorbing traps, in other words, by the presence of large areas free of traps – formula (2). In the opposite limiting case – strong fields, a new asymptotic behavior arises:

$$W(t; E) \propto W_o \exp\left(-\frac{v^2}{4D}t - \frac{3\pi^{1/2}\left(Dt\left[1+\frac{qE}{4ckT}\right]\right)^{1/3}}{2}\right) \tag{13}$$

Let us discuss the obtained results. As follows from expression (16), on large scales and/or in a strong electric field, the probability of particle survival during absorption by traps over long periods of time is determined by a new mechanism – particle drift under the action of an electric field, which is described by the first term in the exponential, and also, along with concentration fluctuations, by drift over a distance of the order of the average distance between absorbing traps, which is described by the second term in the exponential factor.

3. Numerical simulation of the effect of an electric field on particle capture.

The purpose of numerical simulation is to study the behavior and dynamics of particles in two-dimensional space under the influence of an electric field in a

medium with absorbing traps. The simulation is aimed at studying the distribution of particles, as well as establishing the asymptotics of the probability of particle survival in the presence of traps and the effect of the electric field on the time asymptotics. Namely, the effect of the drift mechanism of particle transfer under the influence of an electric field on the probability of their survival when absorbing particles falling on traps was investigated. The model takes into account a number of parameters that directly affect the motion of particles: the direction and intensity of the electric field; the interaction of particles in space; the location of traps; initial conditions. Such a set of parameters allows us to simulate a system in which the electric field creates a drift transfer of particles to absorbing traps, which should lead to an increase in the absorption of particles.

Model and algorithm

To simulate the motion of particles, a model is used that allows us to study the interaction between particles and the electric field and absorbing traps. The model is based on a random walk, in which particles move in discrete steps in four directions, parallel to the coordinate axes, taking into account the influence of the electric field. The electric field in the model is presented as constant and uniformly distributed throughout the space. Its influence sets a directional drift that affects the probability of particle movement. This shift is modeled as an additional probability shift towards the field, which increases the probability of particle movement in one of the directions. The main aspects of the modeling algorithm are described in the Appendix and include: system initialization; particle movement algorithm; absorption check.

Model implementation

The implementation is done in C++, which ensures high performance. To simulate random particle movements, the Mersenne Twister random number generator is used, which has high speed and quality of random sequences, which allows for reliable reproduction of probabilistic particle displacements. Custom classes for working with hash tables have been implemented, which provide quick access to data on particles and traps in space. This structure allows for fast tracking of particles in specific cells, avoiding collisions and ensuring efficient resource management. To speed up the simulation, parallelization is used with OpenMP. Calculations for experiments in a series

are performed in parallel, which significantly reduces the simulation execution time. Flexible settings for the initial system parameters are implemented, such as particle density, electric field intensity, and other parameters. These parameters are configured through configuration files, which allows experimenting with different values without changing the main program code. This implementation allows for easy modification of the interaction rules, for example, introducing new types of traps or adjusting the rules for particle motion under the influence of the field.

Data Visualization and Analysis

The following approaches were used to analyze and visualize the simulation results:

• 2D graphs for particle trajectories: visualizing the motion of particles on a plane allows tracking changes in their positions and the influence of the electric field.

• Density heat maps: displaying the density of particles in each section of space allows identifying clusters caused by the field and areas where movement is slow or difficult.

• Graphs of the change in the probability of movement: allow tracking how the probability of particle movement changes under the influence of the field and over time.

All graphs are made using a program written in Python.

3.1. Simulation results.

An environment with traps was simulated, the traps are randomly distributed within a square measuring 10,000 x 10,000. The concentration of traps is N t = The initial distribution of particles was specified in a circle in the center of coordinates.

Fig. 1a, 1b, 1c show the distribution of particles at the initial moment t= 0 and times t=10,000 and t=100,000.

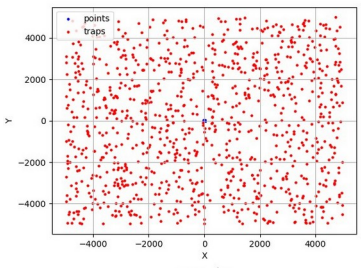
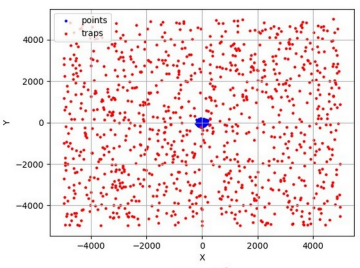


рис. 1а



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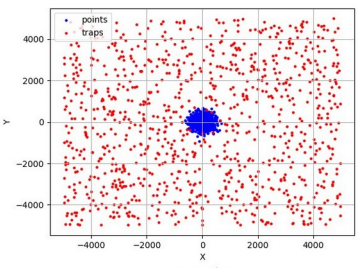


рис. 1в

Fig. 1a) Distribution of particles at moments of time: Fig. 1a) t = 0 Fig. 1b) t = 10000 and Fig. 1c) t = 100000.

The graphs show an obvious diffusion spread of particles and a decrease in the density of traps in the center due to their filling with diffusing particles.

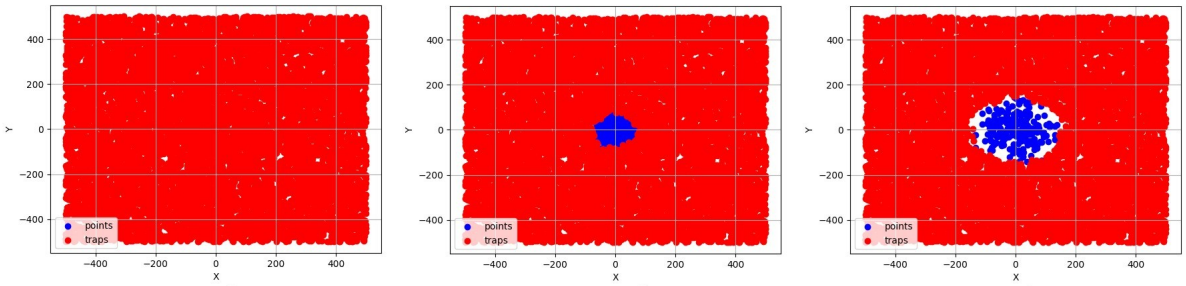


рис. 2а рис. 2б рис. 2в

Fig. 2 also shows the particle distributions in media with traps without an electric field with a higher trap concentration and times 2a) t = 0 and 2b) t = 2000 and 2c) t =25000

Thus, due to the higher trap concentration, the absorption of diffusing particles occurs at a higher rate - and, accordingly, random regions free of traps appear - see Fig. 2c.

Next, the effect of a weak electric field on the particle distributions at different times is investigated. The anisotropy parameter is

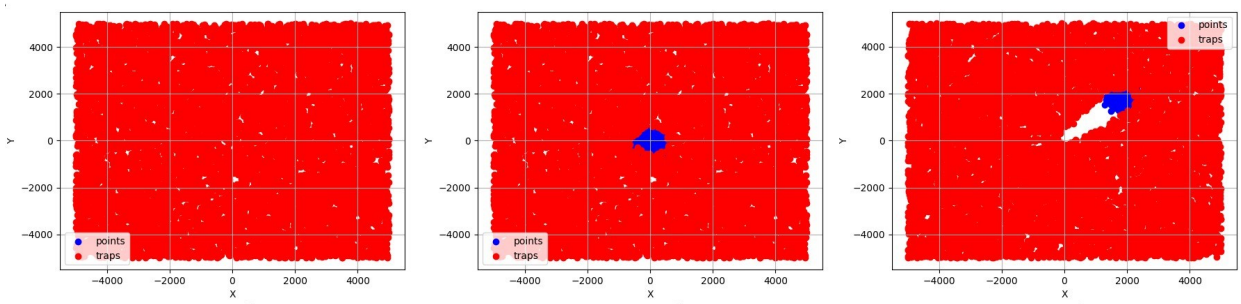


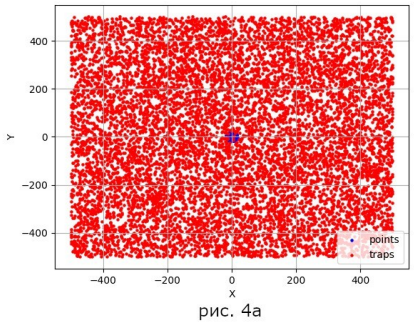
рис. 3а рис. 3б рис. 3в

Figure 3) shows the distribution of particles in an electric field and different times

3a) t = 0 , 3b) t = 10000, 3c) t = 100000.

The influence of weak electric fields manifests itself at large times, when the main transport mechanism becomes drift - particles mainly move along the direction of the electric field and, accordingly, are absorbed along the direction of motion - which can be seen in Figure 3c.

Next, the influence of the electric field in cases of a strong electric field with a large value of the anisotropy parameter was studied. The results are shown in Figure 4.



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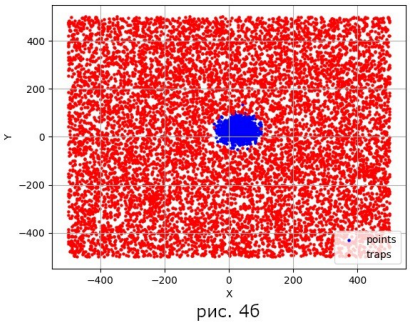

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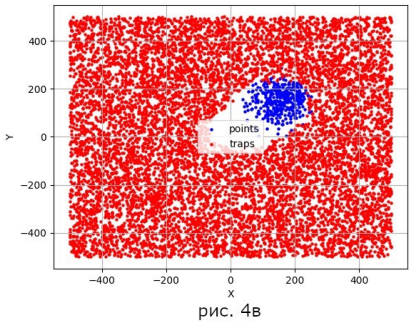
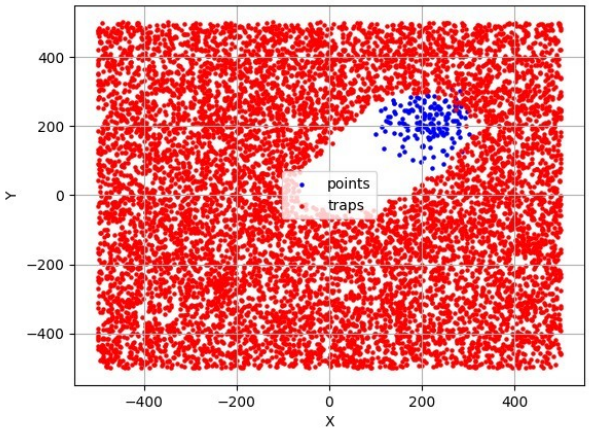


рис. 4в

Fig. 4) shows the distribution of particles in an electric field at different moments of time (Fig. 4a) t = 0, Fig. 4b) t = 2000, Fig. 4c) t = 10000. In the case of strong electric fields, the drift mechanism manifests itself at shorter times - according to (3), the particles shift mainly along the electric field and are absorbed more intensively already at times of 10,000 - see Fig. 4c.



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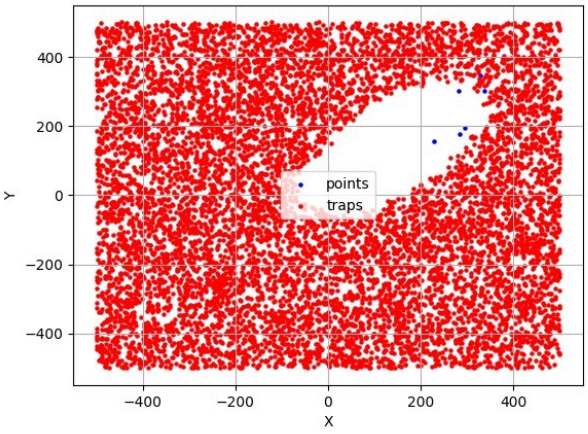

рис. 4д

These figures show the asymptotics of the absorption of a part in an electric field at large times – Fig. 4d) t = 15000 and Fig. 4e) t = 25000.

With increasing time, entire regions of traps filled with diffusing particles appear, stretched along the direction of the electric field.

The results obtained can be presented in the following graphical form:

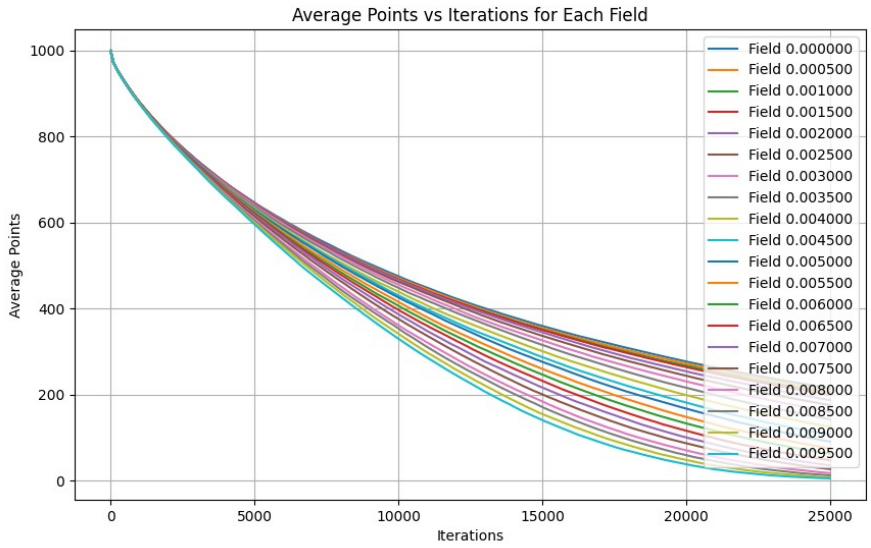

Fig. 5. Graph of the dependence of the decrease in the number of particles on time for different values of the electric field.

According to Fig. 5, the decrease in the number of particles depends on the magnitude of the electric field - the stronger the electric field, the faster the number of particles decreases over time. Approximating the obtained dependencies with an exponential dependence

$$\overline{W}(t; c, E) \propto \exp\left(-\frac{t}{t_{eff}}\right) \tag{14}$$

We obtain numerical values of the effective relaxation time as a function of two variables – the concentration of traps and the magnitude of the anisotropy (electric field)

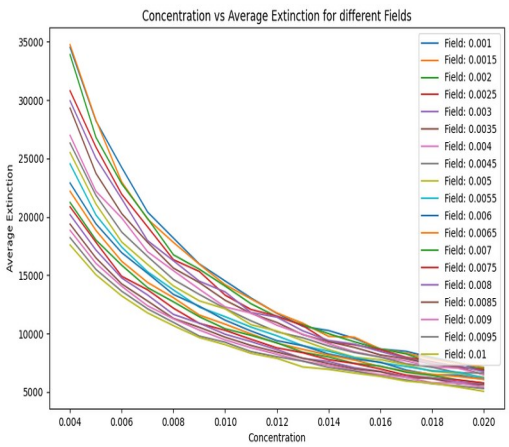

Fig. 6a)

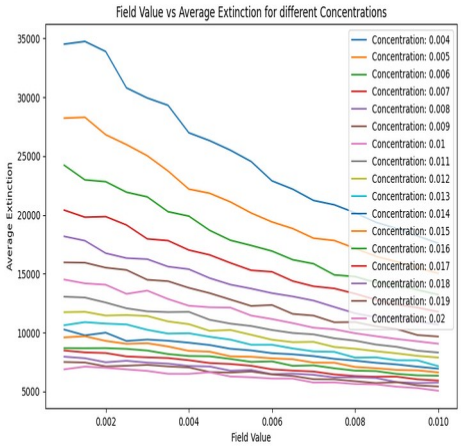

Fig. 6b)

Fig. 6) Dependence of the effective time of decrease in the number of particles on the parameters:

6a) on the concentration of traps at different values of the electric field

6b) on the electric field at different concentrations of traps

However, the obtained results of the dependence of the effective time of decrease can be more clearly presented as a dependence on two variables

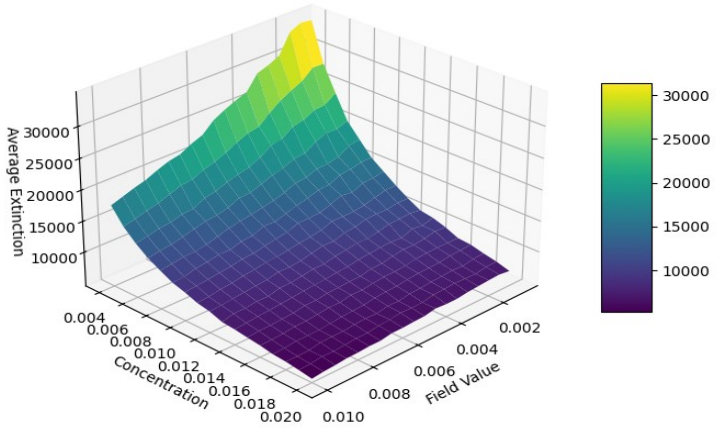

Fig. 7. Effective decay time as a function of two parameters - trap concentration and electric field.

The resulting two-dimensional surface describing the effective relaxation time as a function of two parameters confirms the two-parameter scaling in the problems of particle trapping in an electric field, proposed in [9-11]

4. Conclusion.

Thus, in this paper, the problem of diffusing particle trapping in an electric field is investigated using numerical simulation methods. Asymptotic time dependences of particle survival and the effect of two parameters - trap concentration and electric field strength - on these asymptotics are established. As was shown earlier, in the problem, in accordance with two parameters, two characteristic times arise - the diffusion time over a distance corresponding to the average distance between traps $t_c = (Dc^2)^{-1}$, and the "field" time $t_E = v^2 / D$. Accordingly, by introducing new variables $x = t/t_c; y = t/t_E$, the results obtained above, namely, the logarithm of the probability of particle survival, can be represented as a function of two variables:

$$\ln(W(x,y)/W_0) = -f(x,y) \quad (15)$$

Here $f(x,y)$ is a two-parameter function.

Since in diffusion problems only two characteristic times and, accordingly, two parameters arise and due to the absence of other characteristic parameters, we assume a self-similar nature of the solution to the problem of capturing diffusing particles in an electric field:

$$f(x,y) \propto x^{1/3} g\left(\frac{y}{x}\right) = \begin{cases} x^{1/3}, & 1 << x,\ y << 1 \\ Ay^{1/3}, & 1 << x << y \end{cases} \quad (16)$$

In accordance with the scaling approach in weak electric fields the function depends only on the current time and the capture time on traps $t_c = (Dc^2)^{-1}$, i.e. only on the parameter x in a power-law manner - the upper asymptotics of formula (16). In the case of strong electric fields, when the "field" length $L_E = kT/qE$ becomes less than the distance between traps $L_c = 1/c$: $L_c << L_E$ or in terms of the electric field $1 << qE/kTc$ we obtain a dependence only on the parameter y - the lower asymptotics of formula (16).

This scaling approach indeed corresponds to Fig. 7, and therefore, the numerical simulation of the processes of diffusing particle capture on traps and the influence of the electric field confirms the possibility of developing and using the scaling approach for the problems under study. However, there is also some asymmetry depending on the parameters, namely, a slower decrease in the effective time from the electric field. Apparently, this can be described by introducing the coefficient $A < 1$, but further research is needed to understand the resulting asymmetry. The established asymmetry and fluctuation behavior at large times, which are indicated by both early works [5] and recent studies.

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Appendix A. Description of the model and numerical simulation algorithm.

Model parameters that directly affect the particle motion:

• Direction and intensity of the electric field: the electric field has a directional effect on the particles, causing them to shift more often towards the field. To do this, a constant shift is added to the random particle movements, describing the effect of the electric field.

• Particle interactions in space: particles do not attract or repel each other, but they cannot occupy the same place at the same time. If two particles attempt to move to the same point, they return to their original positions. This constraint simulates the "repulsion" when trying to intersect in space.

• Traps placement: traps are randomly placed in space, which absorb a particle that enters them. Entering a trap leads to the complete disappearance of the particle from the system. The trap locations remain fixed throughout the simulation, which allows us to study the effect of traps on particle survival.

• Initial conditions: the initial positions of the particles and traps determine their initial locations. The density and distribution of traps, as well as the initial positions of the particles, are specified in such a way as to study different scenarios of interactions with traps and drift displacement under the influence of the field. This set of parameters allows us to model a system in which an electric field creates a drift transfer of particles to absorbing traps, which should lead to an increase in the absorption of particles.

The main aspects of the simulation algorithm include the following stages:

• Initialization of the system:

◦ The number of particles is specified. Their initial positions and distribution in space are determined by one of the classes responsible for generating the initial population. This class is selected once before the simulation as one of the system parameters.

◦ The number of traps is specified. Their initial positions and distribution in space are also determined by one of the classes responsible for generating traps. This class is selected once before the simulation as one of the system parameters.

◦ The behavior class of traps is specified, which determines the actions when particles fall into traps.

◦ The simulation time is specified, which determines the number of algorithm iterations. The number of iterations after which the program saves the system configuration is also specified.

◦ The electric field value is specified as a vector. The coordinates of this vector determine the probability of particle displacement in the selected direction.

◦ The algorithm for particle movement and the method of interaction during their collision are specified.

• Particle motion algorithm:

◦ At each time step, one of four directions (along the coordinate axes) is randomly selected for each particle.

◦ The influence of the electric field is taken into account by increasing the probability of motion in the direction of the field.

◦ If two particles try to get to the same position, they "repel" and remain in their previous places.

◦ If more than two particles are involved in a collision, a collision resolution algorithm is used, which first determines all the particles involved in the collision, and then determines the final position for each of them.

• Absorption check:

◦ When a particle hits the coordinates where the trap is located, the particle is removed from the system.

◦ A separate class, defined during system initialization, is responsible for the behavior of the trap.

Model implementation

The implementation is done in C++, which ensures high performance.

To simulate random particle movements, the Mersenne Twister random number generator is used. This generator was chosen due to its high speed and quality of random sequences, which allows for reliable reproduction of probabilistic particle displacements. Custom classes for working with hash tables have been implemented, which provide fast access to data on particles and traps in space. This structure allows for fast tracking of particles in certain cells, avoiding collisions and ensuring efficient resource management.

To speed up the simulation, parallelization is used using OpenMP. Calculations for experiments in a series are performed in parallel, which allows for distributing the load on multithreaded processors and significantly reducing the simulation execution time.

Flexible settings for the initial system parameters have been implemented, such as particle density, electric field intensity, and other parameters. These parameters are easily configured through configuration files, which allows for experimenting with different values without changing the main program code. The implementation allows for easy addition or modification of interaction rules, such as introducing new types of traps or adjusting the rules for particle motion under the influence of the field. Such changes do not require major reworking of the system, which allows for experiments with new conditions and rules.

Data Visualization and Analysis

The following approaches were used to analyze and visualize the simulation results:

• 2D plots for particle trajectories: visualizing particle motion on a plane allows for tracking changes in their positions and the influence of the electric field.

• Density heat maps: displaying the particle density in each section of space allows for identifying field-induced clusters and areas where motion is slow or difficult.

• Movement probability change plots: allow for tracking how the probability of particle motion changes under the influence of the field and over time.

All plots were made using a program written in Python.